Full wwPDB EM Validation Report (i)

Mar 2, 2024 – 09:54 AM EST

PDB ID	:	5URX
EMDB ID	:	EMD-8602
Title	:	Structure of the contracted type VI secretion system sheath in Myxococcus xanthus
Authors	:	Chang, Y.-W.; Rettberg, L.A.; Jensen, G.J.
Deposited on	:	2017-02-13
Resolution	:	28.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

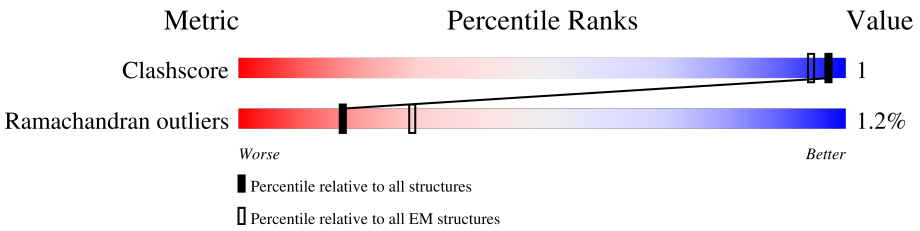
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 28.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	164	9% 80% • 18%
1	1C	164	13% 80% • 18%
1	1E	164	16% 80% • 18%
1	1G	164	13% 80% • 18%
1	1I	164	10% 81% • 18%
1	1K	164	12% 81% • 18%
1	2A	164	11% 80% • 18%
1	2C	164	13% 81% • 18%
1	2E	164	12% 80% • 18%

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Mol	Chain	Length	Quality of chain
1	2G	164	12% 80% • 18%
1	2I	164	14% 80% • 18%
1	2K	164	16% 80% • 18%
1	3A	164	9% 80% • 18%
1	3C	164	11% 80% • 18%
1	3E	164	14% 81% • 18%
1	3G	164	14% 81% • 18%
1	3I	164	15% 80% • 18%
1	3K	164	10% 80% • 18%
2	1B	494	7% 85% • 13%
2	1D	494	6% 85% • 13%
2	1F	494	5% 85% • 13%
2	1H	494	5% 85% • 13%
2	1J	494	6% 86% • 13%
2	1L	494	6% 86% • 13%
2	2B	494	8% 85% • 13%
2	2D	494	5% 86% • 13%
2	2F	494	5% 85% • 13%
2	2H	494	6% 85% • 13%
2	2J	494	6% 85% • 13%
2	2L	494	5% 85% • 13%
2	3B	494	6% 85% • 13%
2	3D	494	7% 85% • 13%
2	3F	494	6% 86% • 13%
2	3H	494	6% 86% • 13%

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Mol	Chain	Length	Quality of chain
2	3J	494	6% 85% • 13%
2	3L	494	5% 85% • 13%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 40752 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called TssB.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	1A	135	540	270	135	135	0	0
1	1C	135	540	270	135	135	0	0
1	1E	135	540	270	135	135	0	0
1	1G	135	540	270	135	135	0	0
1	1I	135	540	270	135	135	0	0
1	1K	135	540	270	135	135	0	0
1	2A	135	540	270	135	135	0	0
1	2C	135	540	270	135	135	0	0
1	2E	135	540	270	135	135	0	0
1	2G	135	540	270	135	135	0	0
1	2I	135	540	270	135	135	0	0
1	2K	135	540	270	135	135	0	0
1	3A	135	540	270	135	135	0	0
1	3C	135	540	270	135	135	0	0
1	3E	135	540	270	135	135	0	0
1	3G	135	540	270	135	135	0	0
1	3I	135	540	270	135	135	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	3K	135	540	270	135	135	0	0

- Molecule 2 is a protein called TssC.

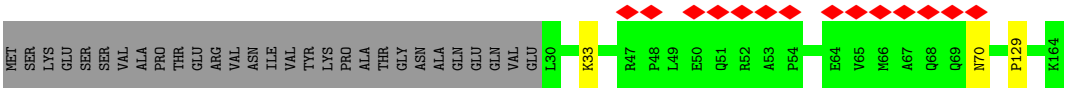
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	1B	431	1724	862	431	431	0	0
2	1D	431	1724	862	431	431	0	0
2	1F	431	1724	862	431	431	0	0
2	1H	431	1724	862	431	431	0	0
2	1J	431	1724	862	431	431	0	0
2	1L	431	1724	862	431	431	0	0
2	2B	431	1724	862	431	431	0	0
2	2D	431	1724	862	431	431	0	0
2	2F	431	1724	862	431	431	0	0
2	2H	431	1724	862	431	431	0	0
2	2J	431	1724	862	431	431	0	0
2	2L	431	1724	862	431	431	0	0
2	3B	431	1724	862	431	431	0	0
2	3D	431	1724	862	431	431	0	0
2	3F	431	1724	862	431	431	0	0
2	3H	431	1724	862	431	431	0	0
2	3J	431	1724	862	431	431	0	0
2	3L	431	1724	862	431	431	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

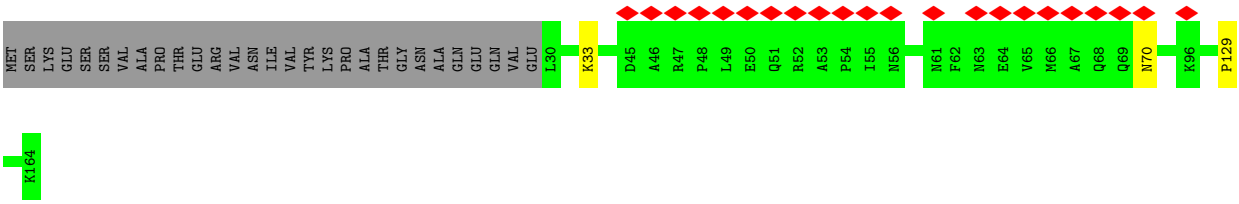
- Molecule 1: TssB

Chain 1A:



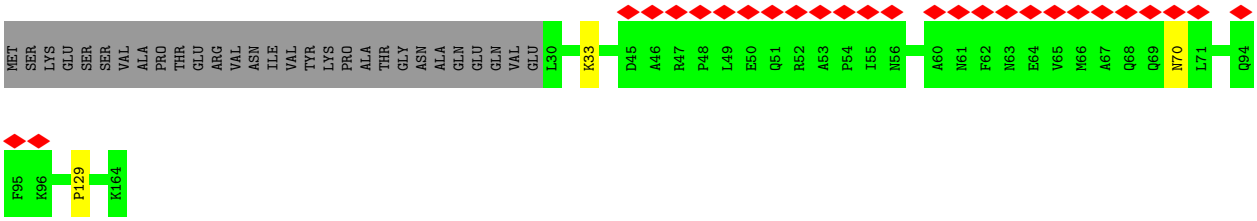
- Molecule 1: TssB

Chain 1C:



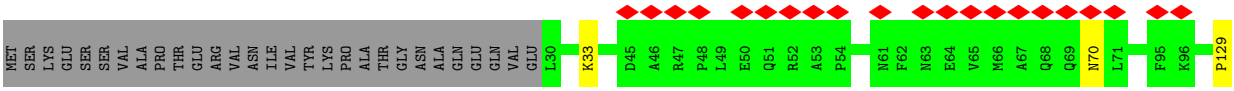
- Molecule 1: TssB

Chain 1E:



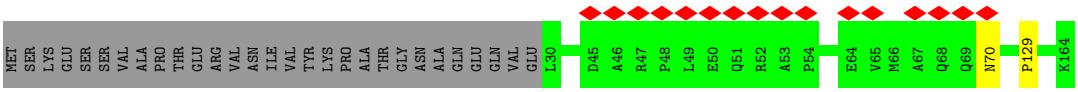
- Molecule 1: TssB

Chain 1G:



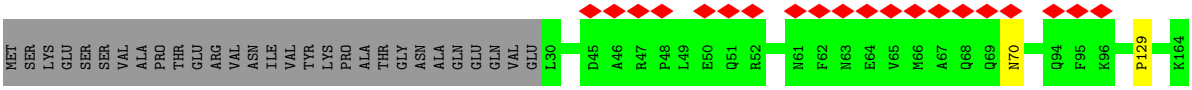
• Molecule 1: TssB

Chain 1I:



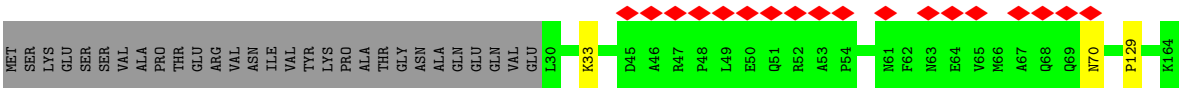
• Molecule 1: TssB

Chain 1K:



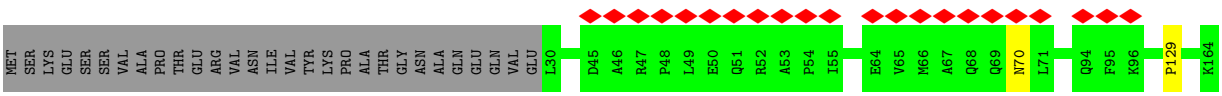
• Molecule 1: TssB

Chain 2A:



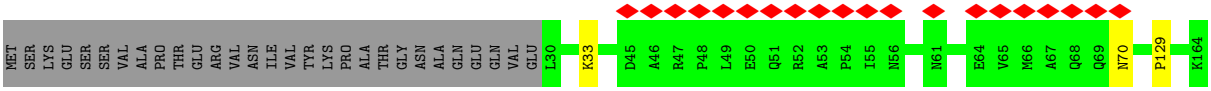
• Molecule 1: TssB

Chain 2C:



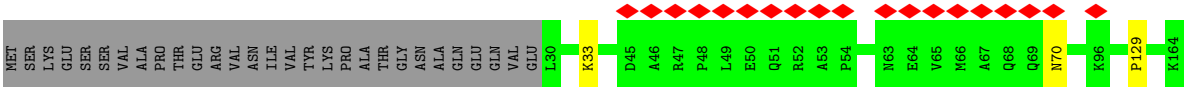
• Molecule 1: TssB

Chain 2E:



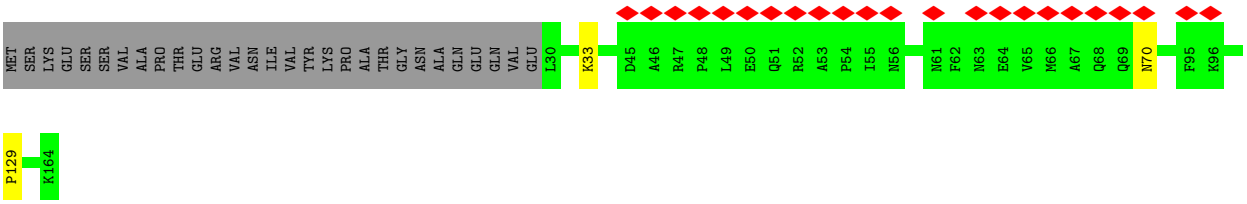
• Molecule 1: TssB

Chain 2G:



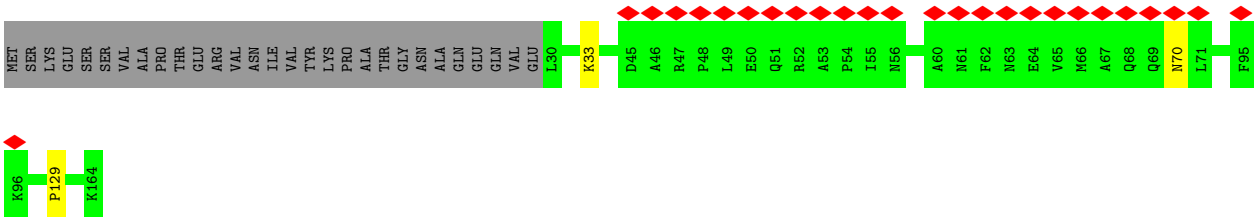
• Molecule 1: TssB

Chain 2I:



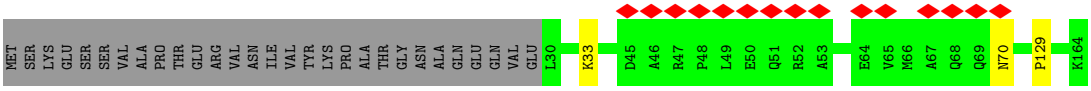
- Molecule 1: TssB

Chain 2K:



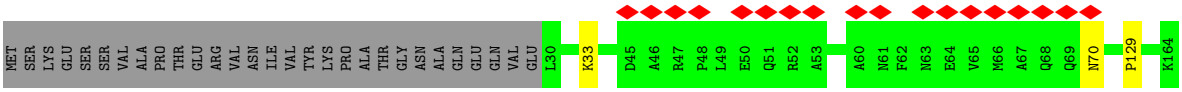
- Molecule 1: TssB

Chain 3A:



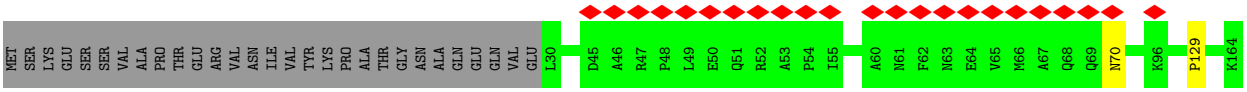
- Molecule 1: TssB

Chain 3C:



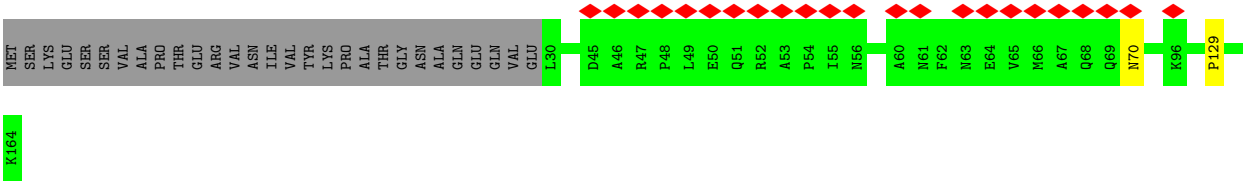
- Molecule 1: TssB

Chain 3E:



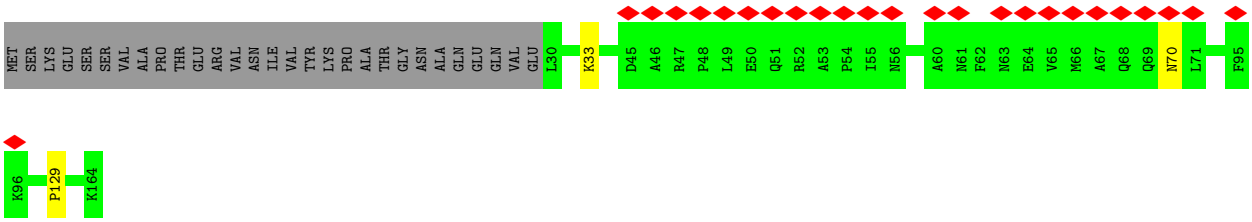
- Molecule 1: TssB

Chain 3G:



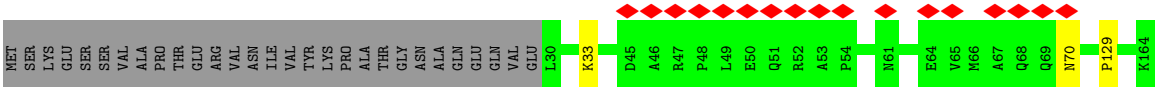
- Molecule 1: TssB

Chain 3I:



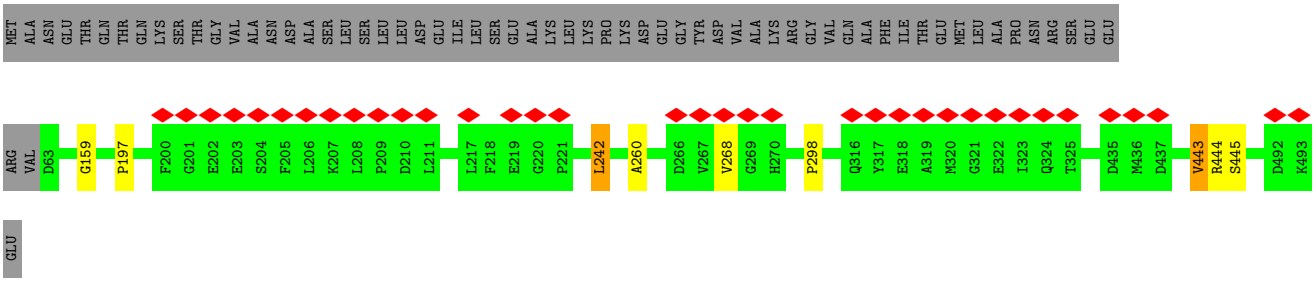
- Molecule 1: TssB

Chain 3K:



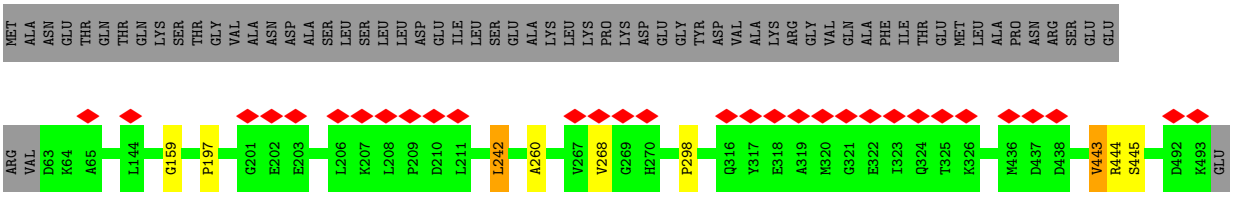
- Molecule 2: TssC

Chain 1B:



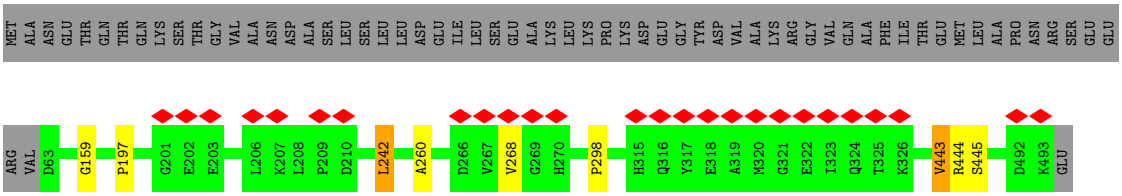
- Molecule 2: TssC

Chain 1D:



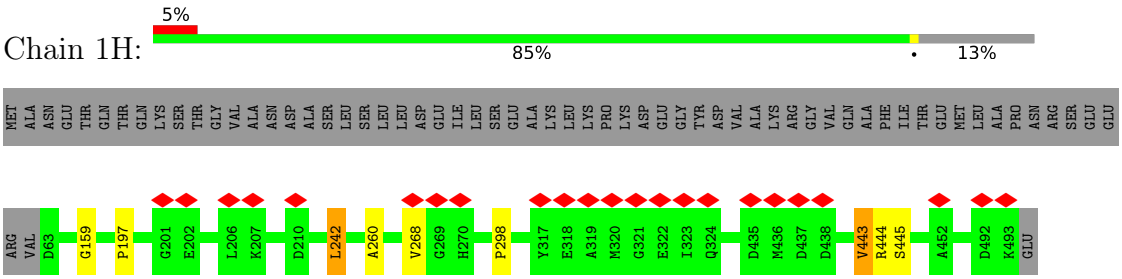
- Molecule 2: TssC

Chain 1F:



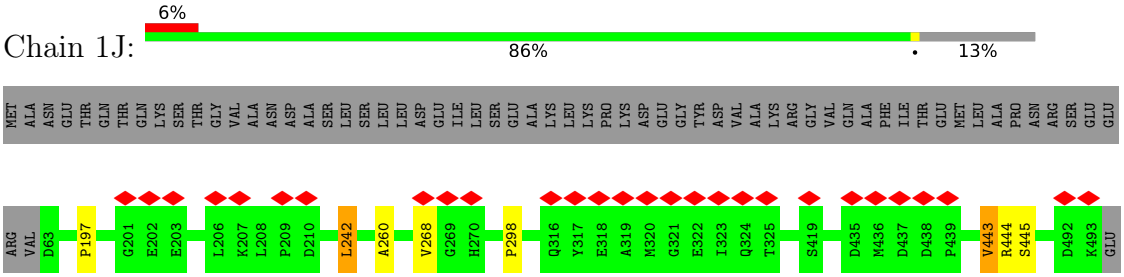
- Molecule 2: TssC

Chain 1H:



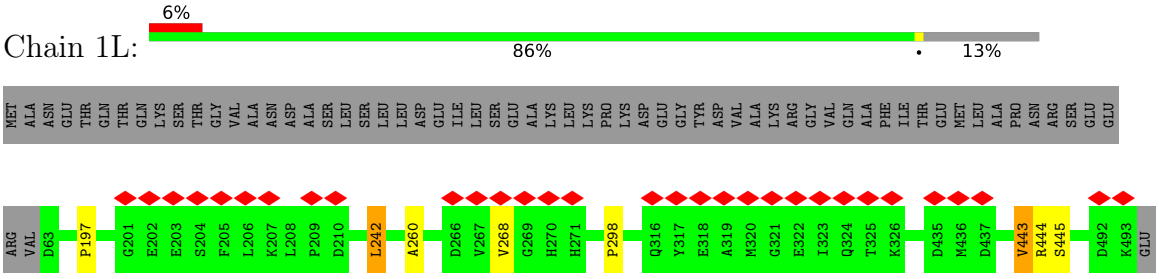
- Molecule 2: TssC

Chain 1J:



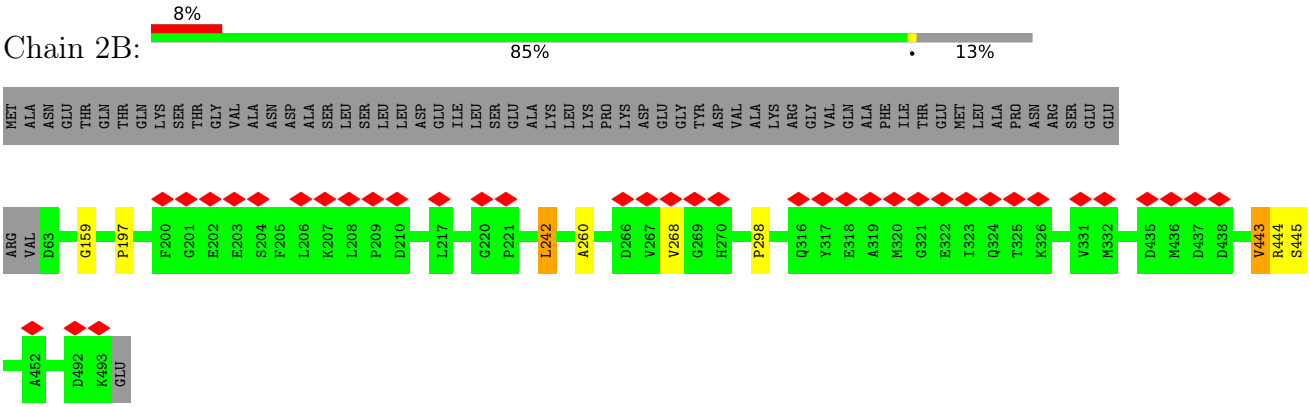
- Molecule 2: TssC

Chain 1L:



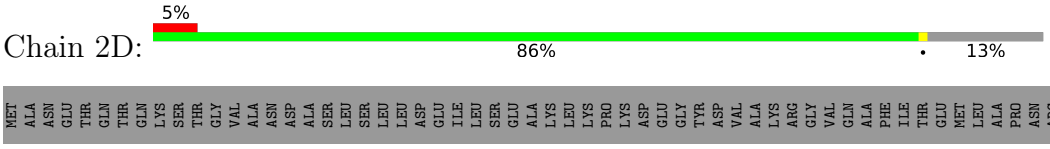
- Molecule 2: TssC

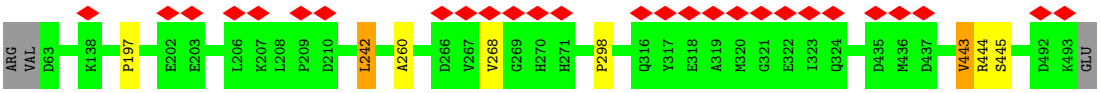
Chain 2B:



- Molecule 2: TssC

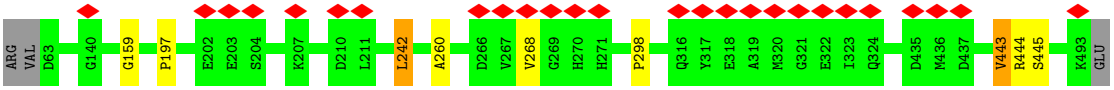
Chain 2D:





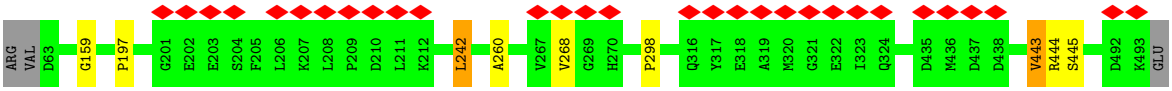
• Molecule 2: TssC

Chain 2F:



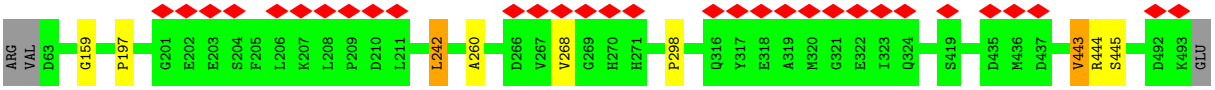
• Molecule 2: TssC

Chain 2H:



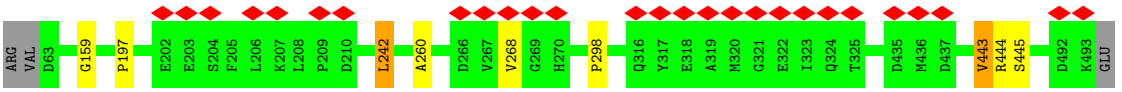
• Molecule 2: TssC

Chain 2J:



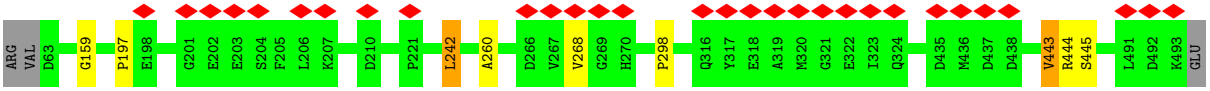
• Molecule 2: TssC

Chain 2L:



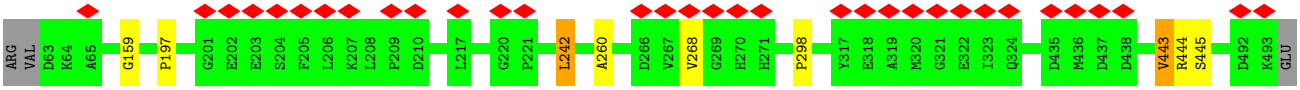
• Molecule 2: TssC

Chain 3B:



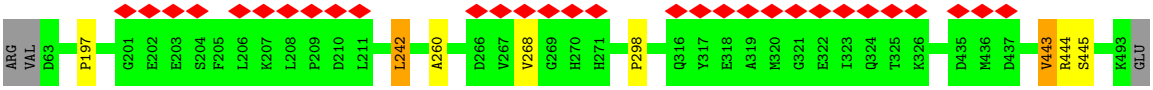
• Molecule 2: TssC

Chain 3D:



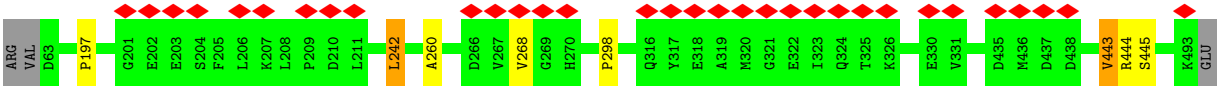
• Molecule 2: TssC

Chain 3F:



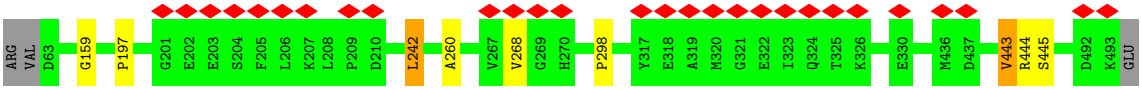
• Molecule 2: TssC

Chain 3H:



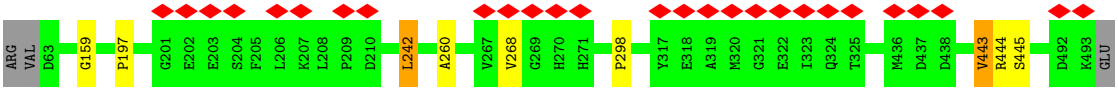
• Molecule 2: TssC

Chain 3J:



• Molecule 2: TssC

Chain 3L:


ARG
VAL
D63
G159
P197
G201
E202
E203
S204
F205
L206
K207
L208
P209
D210
L242
A260
V267
V268
G269
H270
H271
P298
Y317
E318
A319
M320
G321
E322
I323
Q324
T325
M436
D437
D438
V443
R444
S445
D492
K493
GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, Not provided	
Number of subtomograms used	407	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	65535.000	Depositor
Minimum map value	0.001	Depositor
Average map value	32553.326	Depositor
Map value standard deviation	8674.892	Depositor
Recommended contour level	39800.0	Depositor
Map size (Å)	468.00003, 468.0, 468.0	wwPDB
Map dimensions	60, 60, 60	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	7.8000007, 7.8, 7.8	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	1A	0.60	0/539	0.66	0/672
1	1C	0.60	0/539	0.66	0/672
1	1E	0.60	0/539	0.66	0/672
1	1G	0.60	0/539	0.66	0/672
1	1I	0.60	0/539	0.66	0/672
1	1K	0.60	0/539	0.66	0/672
1	2A	0.60	0/539	0.66	0/672
1	2C	0.60	0/539	0.66	0/672
1	2E	0.60	0/539	0.66	0/672
1	2G	0.60	0/539	0.66	0/672
1	2I	0.60	0/539	0.66	0/672
1	2K	0.60	0/539	0.66	0/672
1	3A	0.60	0/539	0.66	0/672
1	3C	0.60	0/539	0.66	0/672
1	3E	0.60	0/539	0.66	0/672
1	3G	0.60	0/539	0.66	0/672
1	3I	0.60	0/539	0.66	0/672
1	3K	0.60	0/539	0.66	0/672
2	1B	0.68	3/1723 (0.2%)	0.72	0/2152
2	1D	0.68	3/1723 (0.2%)	0.72	0/2152
2	1F	0.68	3/1723 (0.2%)	0.72	0/2152
2	1H	0.68	3/1723 (0.2%)	0.72	0/2152
2	1J	0.68	3/1723 (0.2%)	0.72	0/2152
2	1L	0.68	3/1723 (0.2%)	0.72	0/2152
2	2B	0.68	3/1723 (0.2%)	0.72	0/2152
2	2D	0.68	3/1723 (0.2%)	0.72	0/2152
2	2F	0.68	3/1723 (0.2%)	0.72	0/2152
2	2H	0.68	3/1723 (0.2%)	0.72	0/2152
2	2J	0.68	3/1723 (0.2%)	0.72	0/2152
2	2L	0.68	3/1723 (0.2%)	0.72	0/2152
2	3B	0.68	3/1723 (0.2%)	0.72	0/2152
2	3D	0.68	3/1723 (0.2%)	0.72	0/2152
2	3F	0.68	3/1723 (0.2%)	0.72	0/2152
2	3H	0.68	3/1723 (0.2%)	0.72	0/2152

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	3J	0.68	3/1723 (0.2%)	0.72	0/2152
2	3L	0.68	3/1723 (0.2%)	0.72	0/2152
All	All	0.66	54/40716 (0.1%)	0.70	0/50832

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	1B	0	1
2	1D	0	1
2	1F	0	1
2	1H	0	1
2	1J	0	1
2	1L	0	1
2	2B	0	1
2	2D	0	1
2	2F	0	1
2	2H	0	1
2	2J	0	1
2	2L	0	1
2	3B	0	1
2	3D	0	1
2	3F	0	1
2	3H	0	1
2	3J	0	1
2	3L	0	1
All	All	0	18

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2L	242	LEU	C-N	7.51	1.48	1.34
2	1F	242	LEU	C-N	7.49	1.48	1.34
2	3B	242	LEU	C-N	7.49	1.48	1.34
2	3H	242	LEU	C-N	7.48	1.48	1.34
2	1B	242	LEU	C-N	7.48	1.48	1.34
2	2H	242	LEU	C-N	7.47	1.48	1.34
2	3F	242	LEU	C-N	7.47	1.48	1.34
2	1L	242	LEU	C-N	7.46	1.48	1.34
2	2D	242	LEU	C-N	7.45	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2B	242	LEU	C-N	7.45	1.48	1.34
2	2J	242	LEU	C-N	7.44	1.48	1.34
2	1J	242	LEU	C-N	7.44	1.48	1.34
2	1H	242	LEU	C-N	7.43	1.48	1.34
2	3J	242	LEU	C-N	7.43	1.48	1.34
2	1D	242	LEU	C-N	7.42	1.48	1.34
2	3D	242	LEU	C-N	7.41	1.48	1.34
2	3L	242	LEU	C-N	7.41	1.48	1.34
2	2F	242	LEU	C-N	7.40	1.48	1.34
2	2B	242	LEU	C-O	-7.04	1.09	1.23
2	3F	242	LEU	C-O	-7.03	1.09	1.23
2	1J	242	LEU	C-O	-7.02	1.10	1.23
2	2H	242	LEU	C-O	-7.02	1.10	1.23
2	3H	242	LEU	C-O	-7.01	1.10	1.23
2	3L	242	LEU	C-O	-7.00	1.10	1.23
2	2J	242	LEU	C-O	-6.99	1.10	1.23
2	3B	242	LEU	C-O	-6.99	1.10	1.23
2	1F	242	LEU	C-O	-6.98	1.10	1.23
2	2D	242	LEU	C-O	-6.96	1.10	1.23
2	2L	242	LEU	C-O	-6.96	1.10	1.23
2	1B	242	LEU	C-O	-6.96	1.10	1.23
2	1L	242	LEU	C-O	-6.95	1.10	1.23
2	3J	242	LEU	C-O	-6.95	1.10	1.23
2	1D	242	LEU	C-O	-6.94	1.10	1.23
2	1H	242	LEU	C-O	-6.92	1.10	1.23
2	3D	242	LEU	C-O	-6.90	1.10	1.23
2	2F	242	LEU	C-O	-6.87	1.10	1.23
2	1F	197	PRO	C-O	-5.56	1.12	1.23
2	1L	197	PRO	C-O	-5.56	1.12	1.23
2	3B	197	PRO	C-O	-5.55	1.12	1.23
2	3L	197	PRO	C-O	-5.53	1.12	1.23
2	2F	197	PRO	C-O	-5.52	1.12	1.23
2	1H	197	PRO	C-O	-5.50	1.12	1.23
2	3H	197	PRO	C-O	-5.50	1.12	1.23
2	1B	197	PRO	C-O	-5.50	1.12	1.23
2	3J	197	PRO	C-O	-5.50	1.12	1.23
2	2L	197	PRO	C-O	-5.49	1.12	1.23
2	1J	197	PRO	C-O	-5.49	1.12	1.23
2	2H	197	PRO	C-O	-5.48	1.12	1.23
2	3F	197	PRO	C-O	-5.47	1.12	1.23
2	2D	197	PRO	C-O	-5.46	1.12	1.23
2	1D	197	PRO	C-O	-5.45	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2J	197	PRO	C-O	-5.45	1.12	1.23
2	2B	197	PRO	C-O	-5.44	1.12	1.23
2	3D	197	PRO	C-O	-5.43	1.12	1.23

There are no bond angle outliers.

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1B	443	VAL	Peptide
2	1D	443	VAL	Peptide
2	1F	443	VAL	Peptide
2	1H	443	VAL	Peptide
2	1J	443	VAL	Peptide
2	1L	443	VAL	Peptide
2	2B	443	VAL	Peptide
2	2D	443	VAL	Peptide
2	2F	443	VAL	Peptide
2	2H	443	VAL	Peptide
2	2J	443	VAL	Peptide
2	2L	443	VAL	Peptide
2	3B	443	VAL	Peptide
2	3D	443	VAL	Peptide
2	3F	443	VAL	Peptide
2	3H	443	VAL	Peptide
2	3J	443	VAL	Peptide
2	3L	443	VAL	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	540	0	138	1	0
1	1C	540	0	138	1	0
1	1E	540	0	138	1	0
1	1G	540	0	138	1	0
1	1I	540	0	138	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1K	540	0	138	0	0
1	2A	540	0	138	1	0
1	2C	540	0	138	0	0
1	2E	540	0	138	1	0
1	2G	540	0	138	1	0
1	2I	540	0	138	1	0
1	2K	540	0	138	1	0
1	3A	540	0	138	1	0
1	3C	540	0	138	1	0
1	3E	540	0	138	0	0
1	3G	540	0	138	0	0
1	3I	540	0	138	1	0
1	3K	540	0	138	1	0
2	1B	1724	0	462	2	0
2	1D	1724	0	462	2	0
2	1F	1724	0	462	2	0
2	1H	1724	0	462	2	0
2	1J	1724	0	462	1	0
2	1L	1724	0	462	1	0
2	2B	1724	0	462	2	0
2	2D	1724	0	462	1	0
2	2F	1724	0	462	2	0
2	2H	1724	0	462	2	0
2	2J	1724	0	462	2	0
2	2L	1724	0	462	2	0
2	3B	1724	0	462	2	0
2	3D	1724	0	462	2	0
2	3F	1724	0	462	1	0
2	3H	1724	0	462	1	0
2	3J	1724	0	462	2	0
2	3L	1724	0	462	2	0
All	All	40752	0	10800	31	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (31) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2H:443:VAL:C	2:2H:445:SER:N	2.71	0.44
2:1B:443:VAL:C	2:1B:445:SER:N	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1F:443:VAL:C	2:1F:445:SER:N	2.72	0.44
1:1G:33:LYS:O	2:1H:159:GLY:N	2.48	0.44
2:3D:443:VAL:C	2:3D:445:SER:N	2.72	0.44
2:1H:443:VAL:C	2:1H:445:SER:N	2.72	0.43
2:3L:443:VAL:C	2:3L:445:SER:N	2.72	0.43
2:2F:443:VAL:C	2:2F:445:SER:N	2.72	0.43
2:2L:443:VAL:C	2:2L:445:SER:N	2.71	0.43
2:3B:443:VAL:C	2:3B:445:SER:N	2.72	0.43
2:3F:443:VAL:C	2:3F:445:SER:N	2.71	0.43
2:2B:443:VAL:C	2:2B:445:SER:N	2.72	0.43
1:2A:33:LYS:O	2:2B:159:GLY:N	2.48	0.43
2:2J:443:VAL:C	2:2J:445:SER:N	2.71	0.43
1:3A:33:LYS:O	2:3B:159:GLY:N	2.48	0.43
2:2D:443:VAL:C	2:2D:445:SER:N	2.71	0.43
2:3J:443:VAL:C	2:3J:445:SER:N	2.72	0.43
1:3K:33:LYS:O	2:3L:159:GLY:N	2.48	0.43
2:1L:443:VAL:C	2:1L:445:SER:N	2.72	0.43
1:1C:33:LYS:O	2:1D:159:GLY:N	2.48	0.43
2:3H:443:VAL:C	2:3H:445:SER:N	2.72	0.42
1:1A:33:LYS:O	2:1B:159:GLY:N	2.48	0.42
2:1J:443:VAL:C	2:1J:445:SER:N	2.71	0.42
2:1D:443:VAL:C	2:1D:445:SER:N	2.71	0.42
1:2E:33:LYS:O	2:2F:159:GLY:N	2.48	0.41
1:2I:33:LYS:O	2:2J:159:GLY:N	2.48	0.41
1:2G:33:LYS:O	2:2H:159:GLY:N	2.48	0.41
1:2K:33:LYS:O	2:2L:159:GLY:N	2.48	0.41
1:3I:33:LYS:O	2:3J:159:GLY:N	2.48	0.41
1:3C:33:LYS:O	2:3D:159:GLY:N	2.48	0.41
1:1E:33:LYS:O	2:1F:159:GLY:N	2.48	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	10	46
1	1C	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	10	46
1	1E	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	10	46
1	1G	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	10	46
1	1I	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	10	46
1	1K	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	10	46
1	2A	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	10	46
1	2C	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	10	46
1	2E	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	10	46
1	2G	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	10	46
1	2I	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	10	46
1	2K	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	10	46
1	3A	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	10	46
1	3C	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	10	46
1	3E	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	10	46
1	3G	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	10	46
1	3I	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	10	46
1	3K	133/164 (81%)	128 (96%)	3 (2%)	2 (2%)	10	46
2	1B	429/494 (87%)	403 (94%)	21 (5%)	5 (1%)	13	50
2	1D	429/494 (87%)	402 (94%)	22 (5%)	5 (1%)	13	50
2	1F	429/494 (87%)	402 (94%)	22 (5%)	5 (1%)	13	50
2	1H	429/494 (87%)	402 (94%)	22 (5%)	5 (1%)	13	50
2	1J	429/494 (87%)	403 (94%)	21 (5%)	5 (1%)	13	50
2	1L	429/494 (87%)	403 (94%)	21 (5%)	5 (1%)	13	50
2	2B	429/494 (87%)	402 (94%)	22 (5%)	5 (1%)	13	50
2	2D	429/494 (87%)	403 (94%)	21 (5%)	5 (1%)	13	50
2	2F	429/494 (87%)	402 (94%)	22 (5%)	5 (1%)	13	50
2	2H	429/494 (87%)	402 (94%)	22 (5%)	5 (1%)	13	50
2	2J	429/494 (87%)	403 (94%)	21 (5%)	5 (1%)	13	50
2	2L	429/494 (87%)	402 (94%)	22 (5%)	5 (1%)	13	50
2	3B	429/494 (87%)	402 (94%)	22 (5%)	5 (1%)	13	50
2	3D	429/494 (87%)	402 (94%)	22 (5%)	5 (1%)	13	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	3F	429/494 (87%)	404 (94%)	20 (5%)	5 (1%)	13	50
2	3H	429/494 (87%)	403 (94%)	21 (5%)	5 (1%)	13	50
2	3J	429/494 (87%)	402 (94%)	22 (5%)	5 (1%)	13	50
2	3L	429/494 (87%)	402 (94%)	22 (5%)	5 (1%)	13	50
All	All	10116/11844 (85%)	9548 (94%)	442 (4%)	126 (1%)	17	50

All (126) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1A	129	PRO
2	1B	242	LEU
2	1B	444	ARG
1	1C	129	PRO
2	1D	242	LEU
2	1D	444	ARG
1	1E	129	PRO
2	1F	242	LEU
2	1F	444	ARG
1	1G	129	PRO
2	1H	242	LEU
2	1H	444	ARG
1	1I	129	PRO
2	1J	242	LEU
2	1J	444	ARG
1	1K	129	PRO
2	1L	242	LEU
2	1L	444	ARG
1	2A	129	PRO
2	2B	242	LEU
2	2B	444	ARG
1	2C	129	PRO
2	2D	242	LEU
2	2D	444	ARG
1	2E	129	PRO
2	2F	242	LEU
2	2F	444	ARG
1	2G	129	PRO
2	2H	242	LEU
2	2H	444	ARG
1	2I	129	PRO
2	2J	242	LEU

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Mol	Chain	Res	Type
2	2J	444	ARG
1	2K	129	PRO
2	2L	242	LEU
2	2L	444	ARG
1	3A	129	PRO
2	3B	242	LEU
2	3B	444	ARG
1	3C	129	PRO
2	3D	242	LEU
2	3D	444	ARG
1	3E	129	PRO
2	3F	242	LEU
2	3F	444	ARG
1	3G	129	PRO
2	3H	242	LEU
2	3H	444	ARG
1	3I	129	PRO
2	3J	242	LEU
2	3J	444	ARG
1	3K	129	PRO
2	3L	242	LEU
2	3L	444	ARG
2	1B	260	ALA
2	1B	268	VAL
2	1D	260	ALA
2	1D	268	VAL
2	1F	260	ALA
2	1F	268	VAL
2	1H	260	ALA
2	1H	268	VAL
2	1J	260	ALA
2	1J	268	VAL
2	1L	260	ALA
2	1L	268	VAL
2	2B	260	ALA
2	2B	268	VAL
2	2D	260	ALA
2	2D	268	VAL
2	2F	260	ALA
2	2F	268	VAL
2	2H	260	ALA
2	2H	268	VAL

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Mol	Chain	Res	Type
2	2J	260	ALA
2	2J	268	VAL
2	2L	260	ALA
2	2L	268	VAL
2	3B	260	ALA
2	3B	268	VAL
2	3D	260	ALA
2	3D	268	VAL
2	3F	260	ALA
2	3F	268	VAL
2	3H	260	ALA
2	3H	268	VAL
2	3J	260	ALA
2	3J	268	VAL
2	3L	260	ALA
2	3L	268	VAL
1	1A	70	ASN
1	1C	70	ASN
1	1E	70	ASN
1	1G	70	ASN
1	1I	70	ASN
1	1K	70	ASN
1	2A	70	ASN
1	2C	70	ASN
1	2E	70	ASN
1	2G	70	ASN
1	2I	70	ASN
1	2K	70	ASN
1	3A	70	ASN
1	3C	70	ASN
1	3E	70	ASN
1	3G	70	ASN
1	3I	70	ASN
1	3K	70	ASN
2	1B	298	PRO
2	1D	298	PRO
2	1F	298	PRO
2	1H	298	PRO
2	1J	298	PRO
2	1L	298	PRO
2	2B	298	PRO
2	2D	298	PRO

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Mol	Chain	Res	Type
2	2F	298	PRO
2	2H	298	PRO
2	2J	298	PRO
2	2L	298	PRO
2	3B	298	PRO
2	3D	298	PRO
2	3F	298	PRO
2	3H	298	PRO
2	3J	298	PRO
2	3L	298	PRO

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

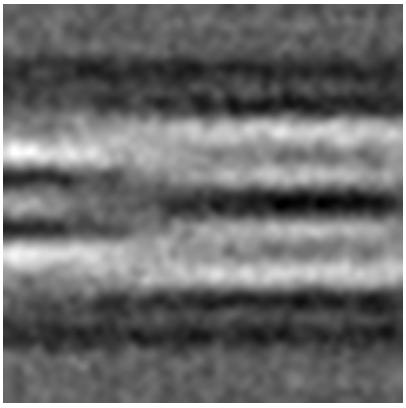
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-8602. These allow visual inspection of the internal detail of the map and identification of artifacts.

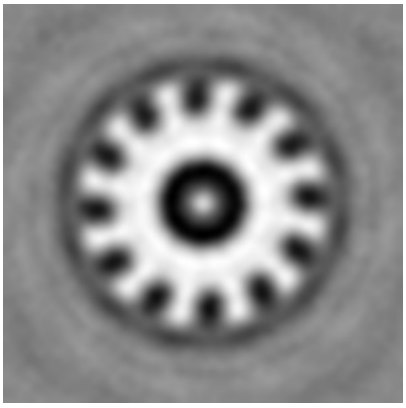
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

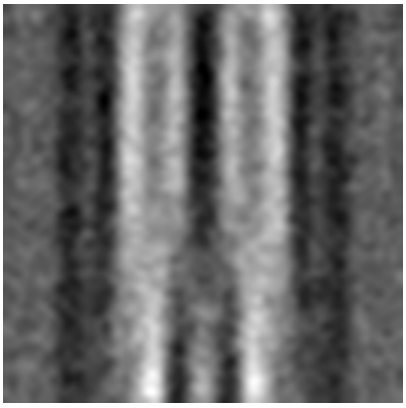
6.1.1 Primary map



X



Y

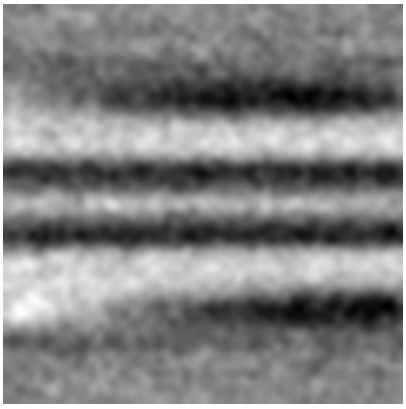


Z

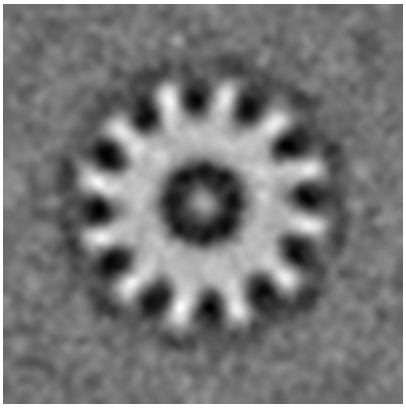
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

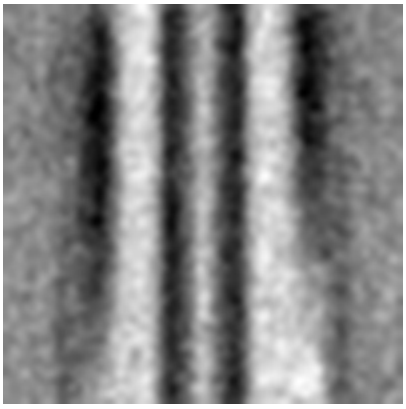
6.2.1 Primary map



X Index: 30



Y Index: 30

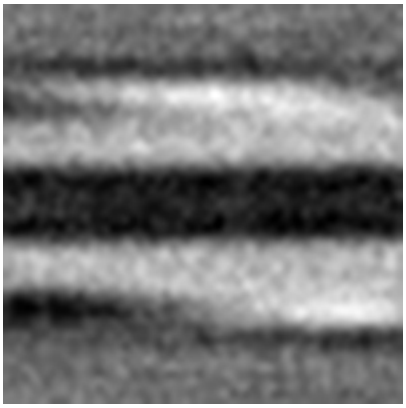


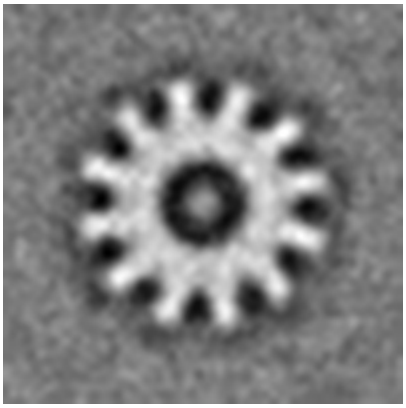
Z Index: 30

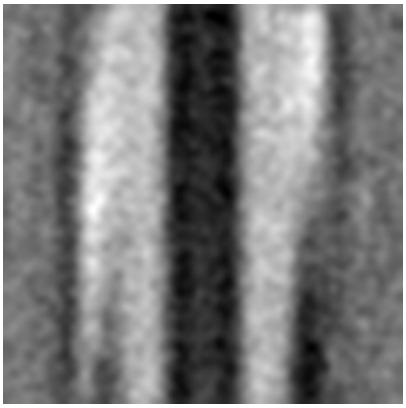
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 26

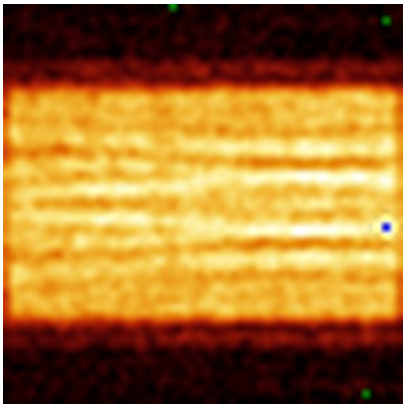

Y Index: 57

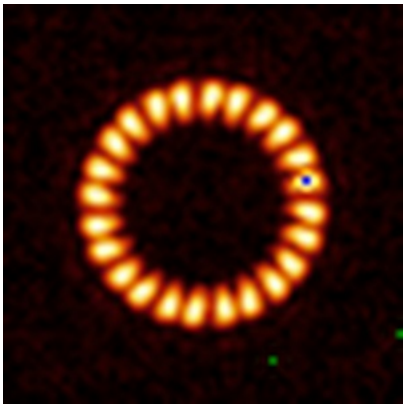

Z Index: 26

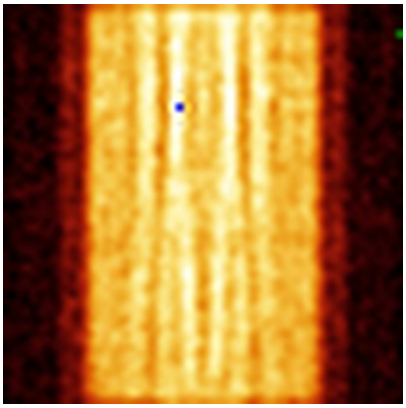
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map


X

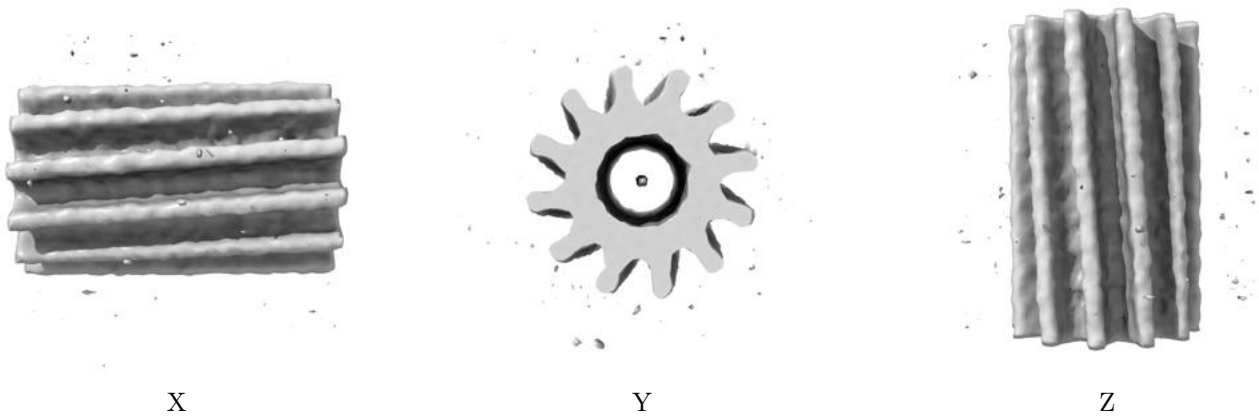

Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 39800.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

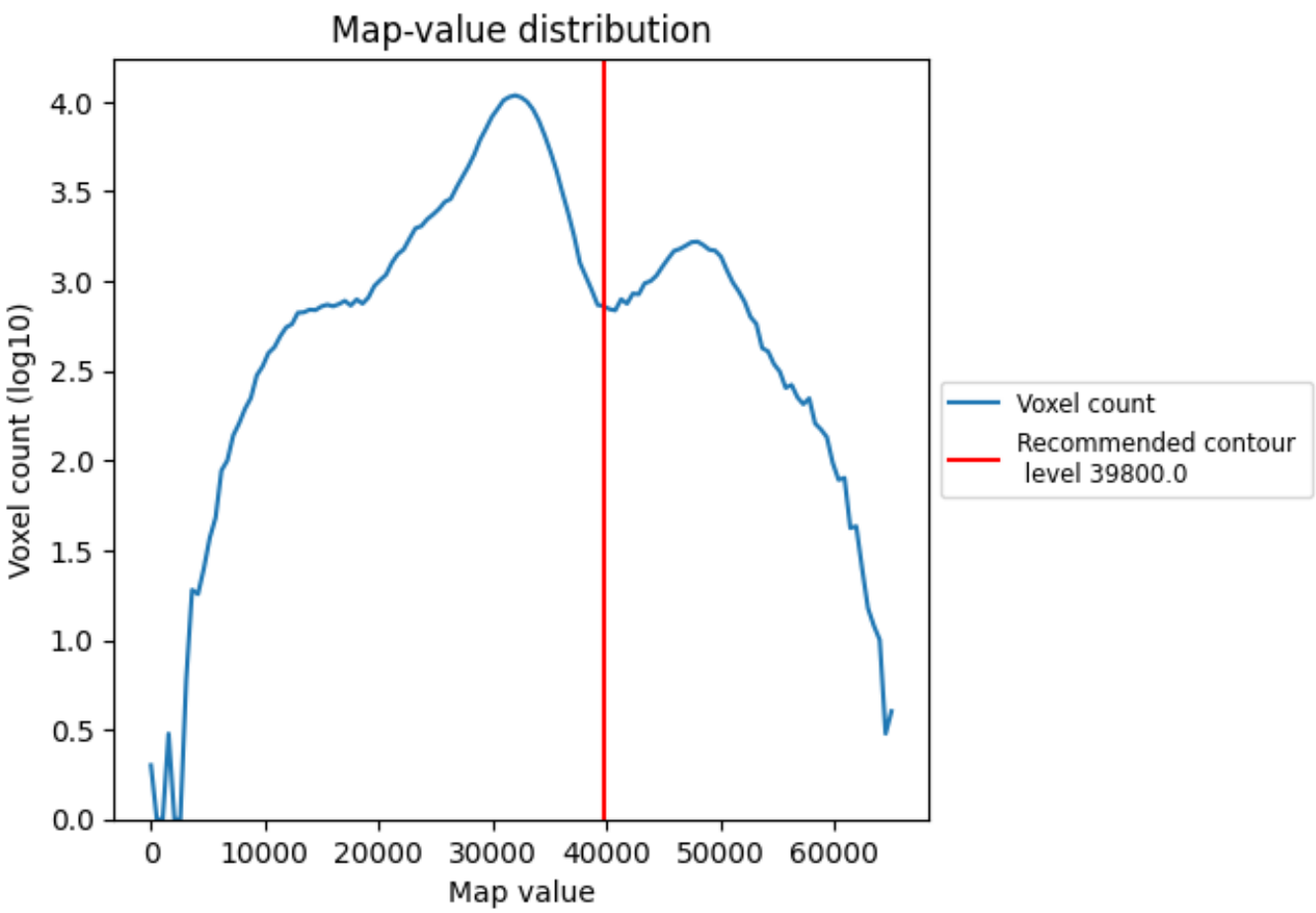
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

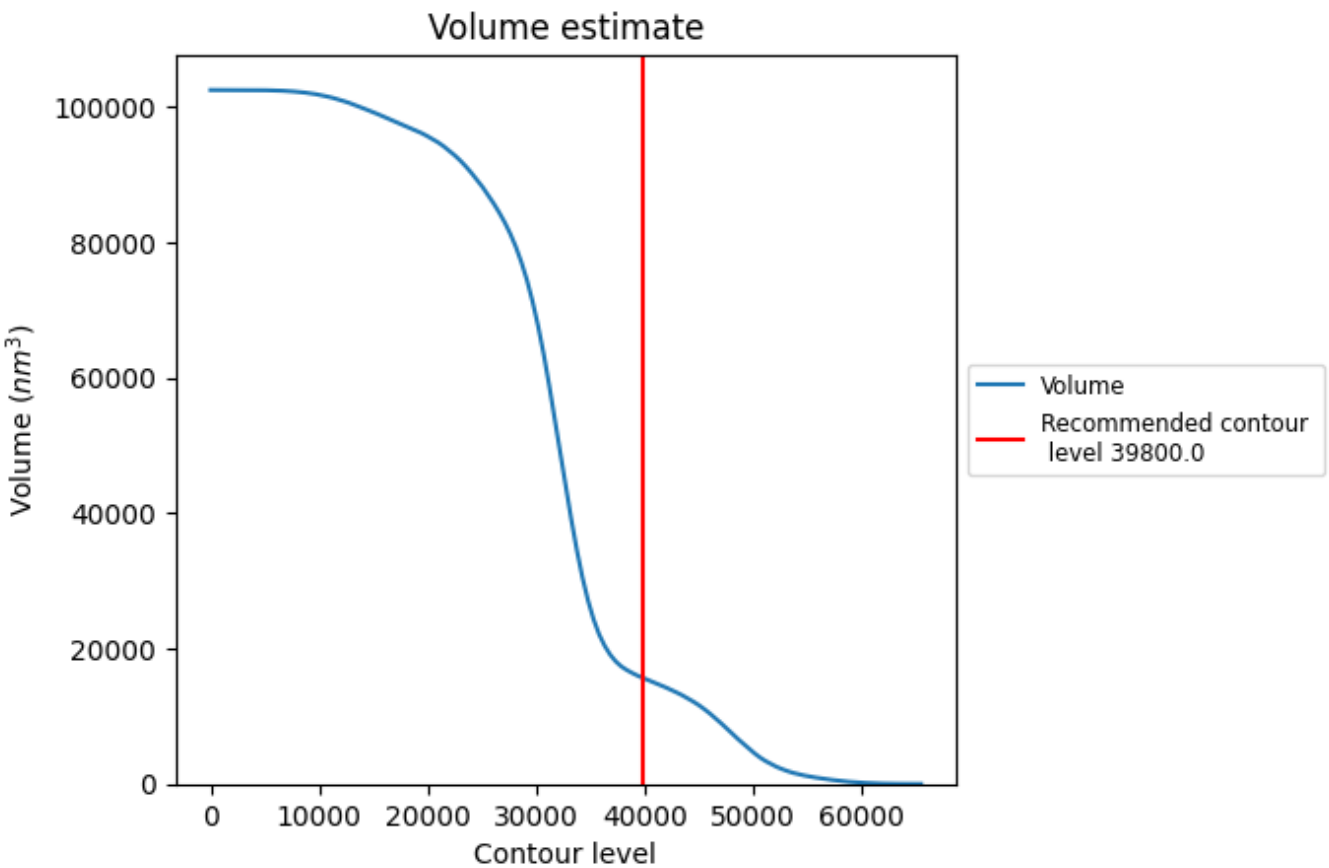
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

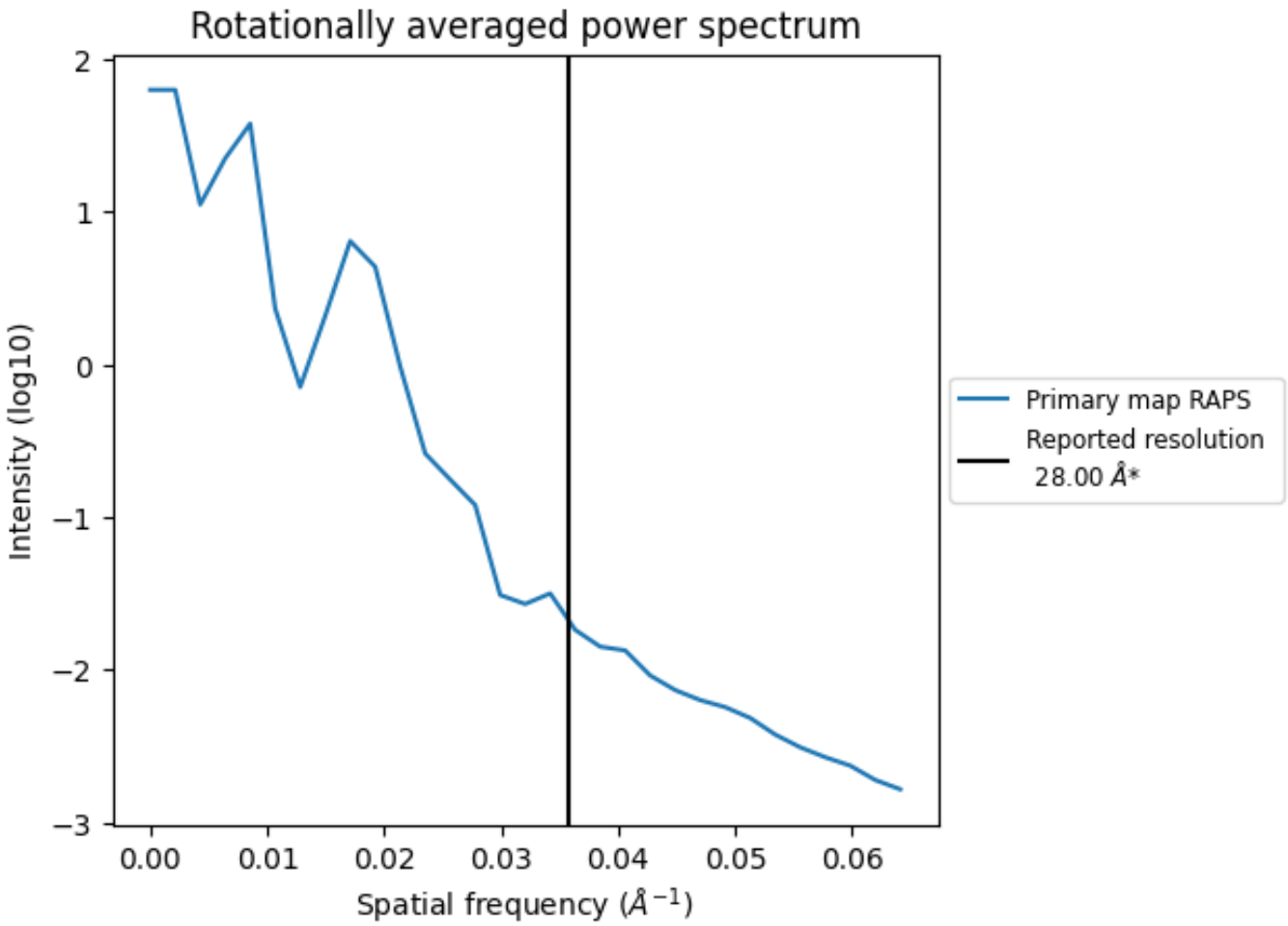
7.2 Volume estimate (i)



The volume at the recommended contour level is 15723 nm^3; this corresponds to an approximate mass of 14203 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.036 Å^{-1}

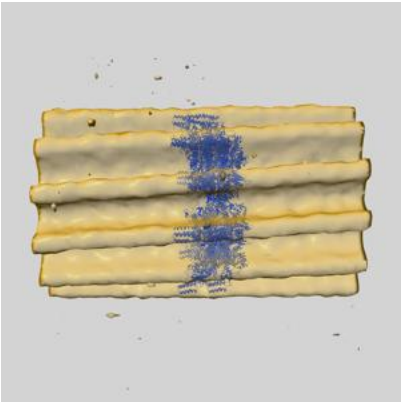
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

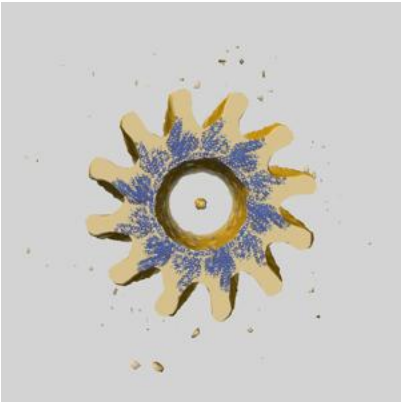
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-8602 and PDB model 5URX. Per-residue inclusion information can be found in section 3 on page 7.

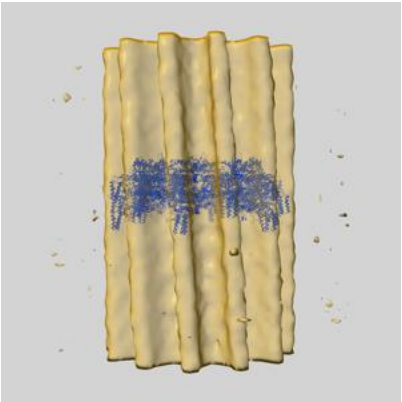
9.1 Map-model overlay (i)



X



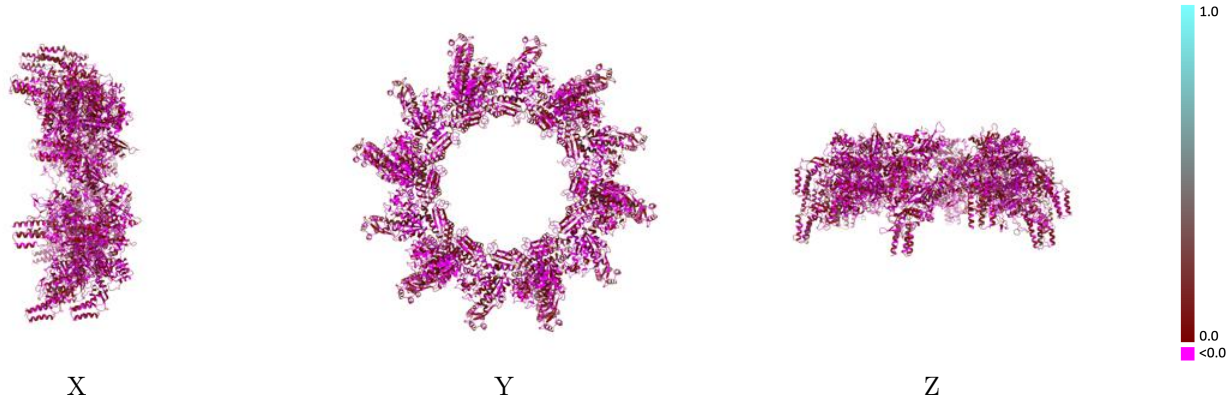
Y



Z

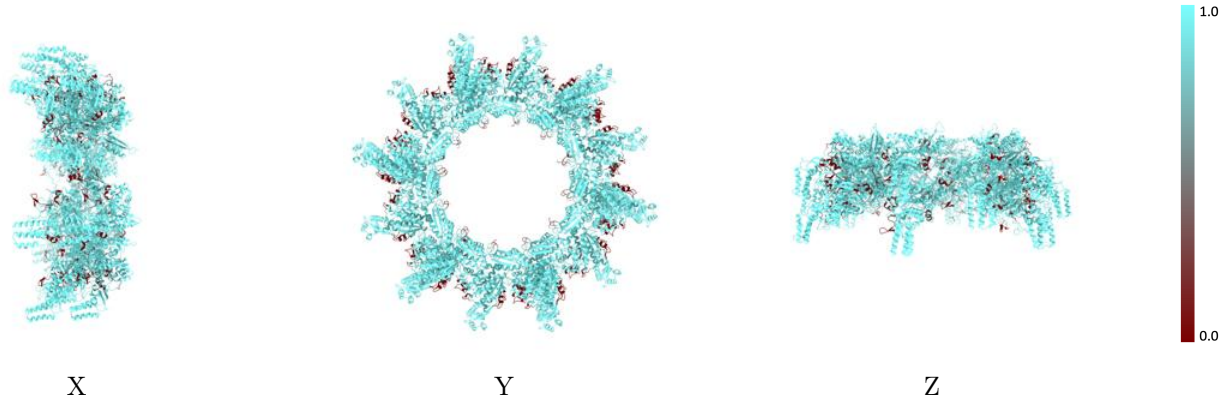
The images above show the 3D surface view of the map at the recommended contour level 39800.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



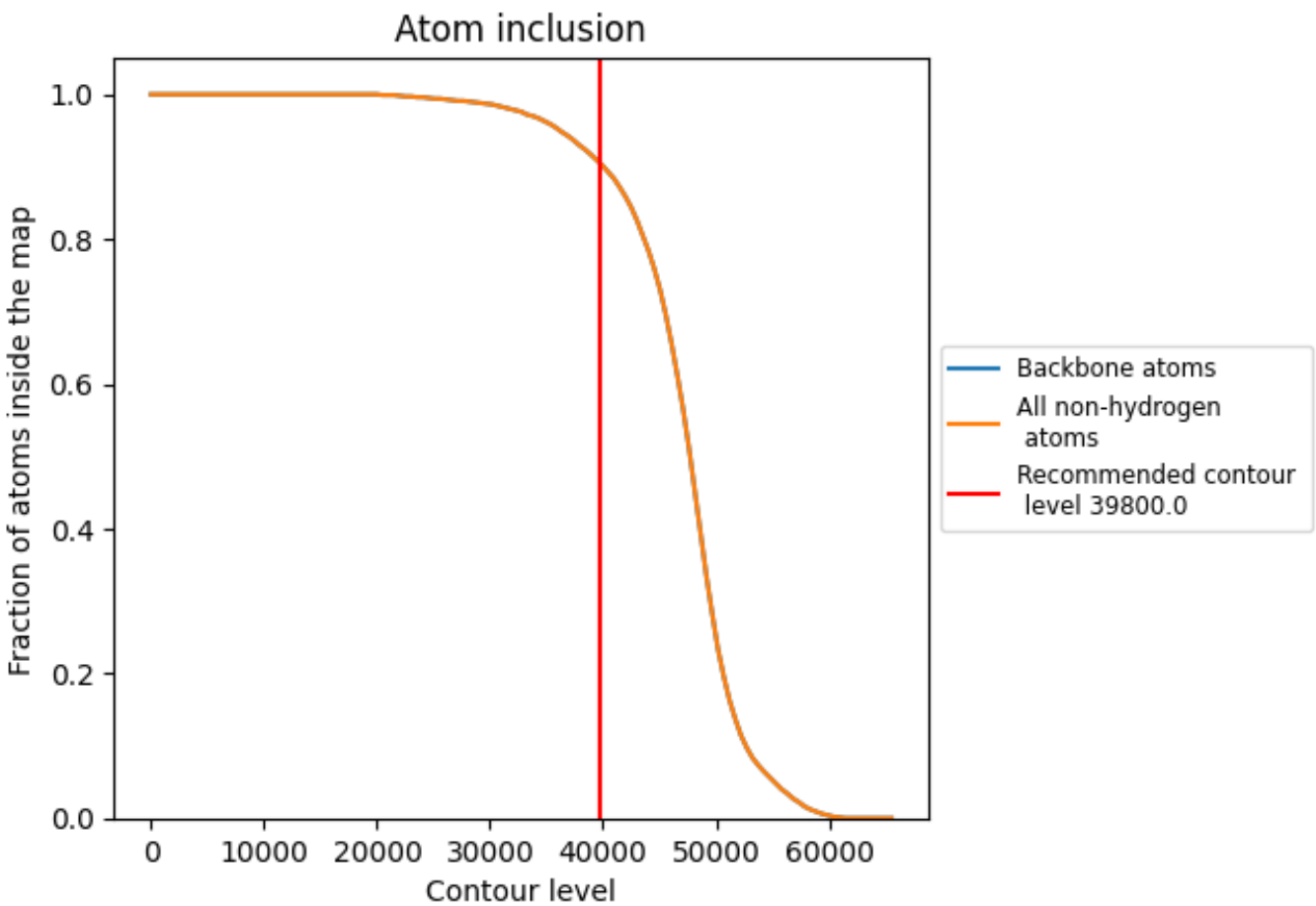
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (39800.0).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (39800.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9040	0.0280
1A	0.8810	0.0530
1B	0.9100	0.0280
1C	0.8260	0.0300
1D	0.9200	0.0250
1E	0.7830	0.0540
1F	0.9330	0.0190
1G	0.8390	0.0420
1H	0.9390	0.0160
1I	0.8650	0.0320
1J	0.9250	0.0180
1K	0.8390	0.0420
1L	0.9250	0.0100
2A	0.8650	0.0590
2B	0.9030	0.0190
2C	0.8190	0.0660
2D	0.9290	0.0190
2E	0.8410	0.0450
2F	0.9360	0.0210
2G	0.8440	0.0520
2H	0.9300	0.0220
2I	0.8200	0.0520
2J	0.9260	0.0250
2K	0.8040	0.0160
2L	0.9330	0.0220
3A	0.8760	0.0620
3B	0.9200	0.0250
3C	0.8690	0.0740
3D	0.9140	0.0220
3E	0.8300	0.0680
3F	0.9250	0.0220
3G	0.8370	0.0430
3H	0.9230	0.0240
3I	0.8090	0.0350
3J	0.9270	0.0190

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Chain	Atom inclusion	Q-score
3K	0.8570	0.0410
3L	0.9280	0.0320